



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:31 AM UTC

PDB ID : 5VHR / pdb_00005vhr
EMDB ID : EMD-8683
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2017-04-13
Resolution : 7.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

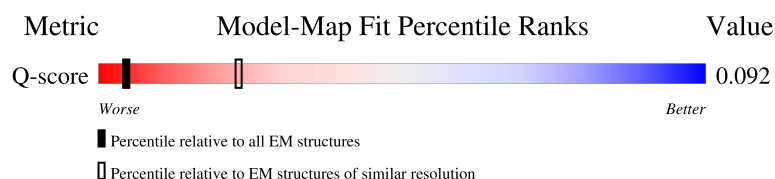
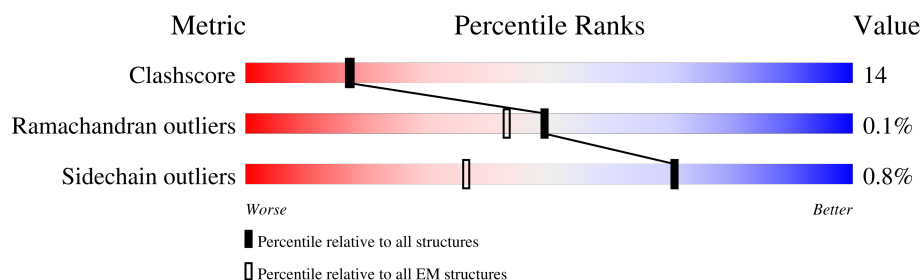
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	384 (7.20 - 8.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	223	26% 67% 22% 11%
2	A	266	22% 70% 27% .
3	B	267	19% 70% 17% 13%
4	D	262	37% 68% 22% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	262	25% 56% 24% 20%
6	F	267	17% 65% 30% 6%
7	C	266	39% 65% 25% 9%
8	f	848	10% 52% 28% 19%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18057 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	199	Total	C	N	O	S	0	0
			1516	945	266	297	8		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	258	Total	C	N	O	S	0	0
			2022	1271	365	371	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	233	Total	C	N	O	S	0	0
			1843	1163	318	354	8		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1873	1184	332	348	9		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1644	1032	294	306	12		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	252	Total	C	N	O	S	0	0
			1965	1232	348	371	14		

- Molecule 7 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	242	Total	C	N	O	S	0	0
			1890	1190	337	350	13		

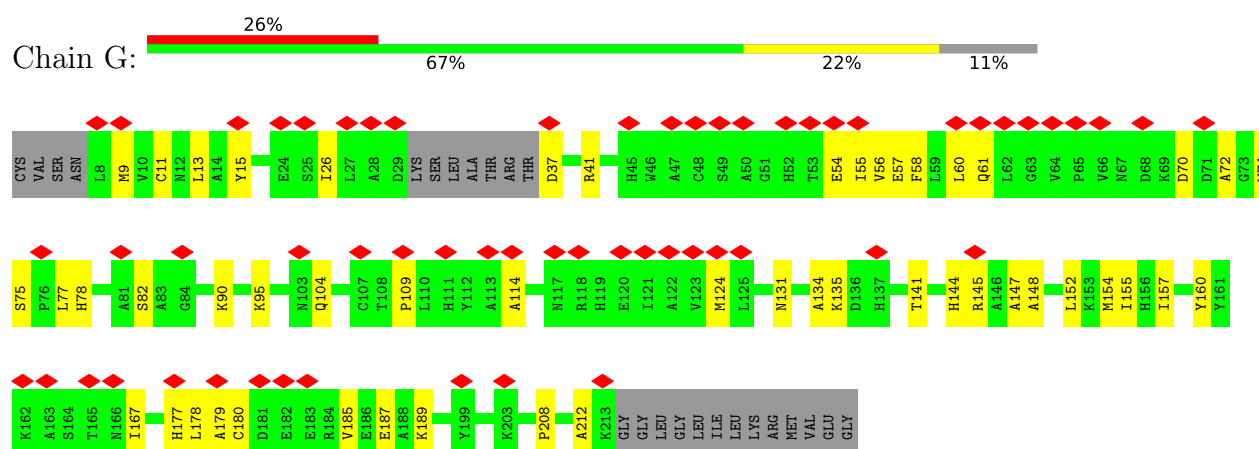
- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	686	Total	C	N	O	S	0	0
			5304	3335	901	1033	35		

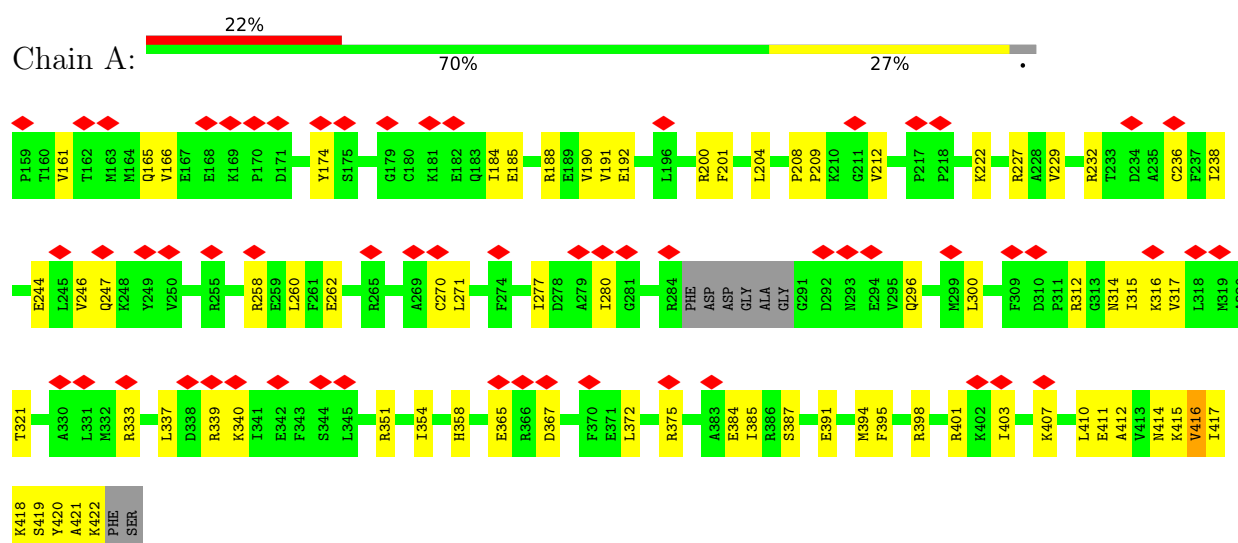
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10

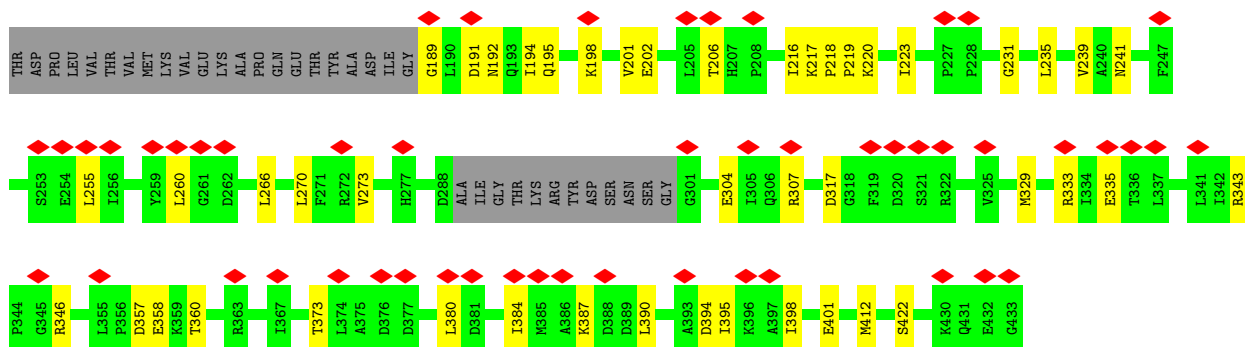


- Molecule 2: 26S proteasome regulatory subunit 7

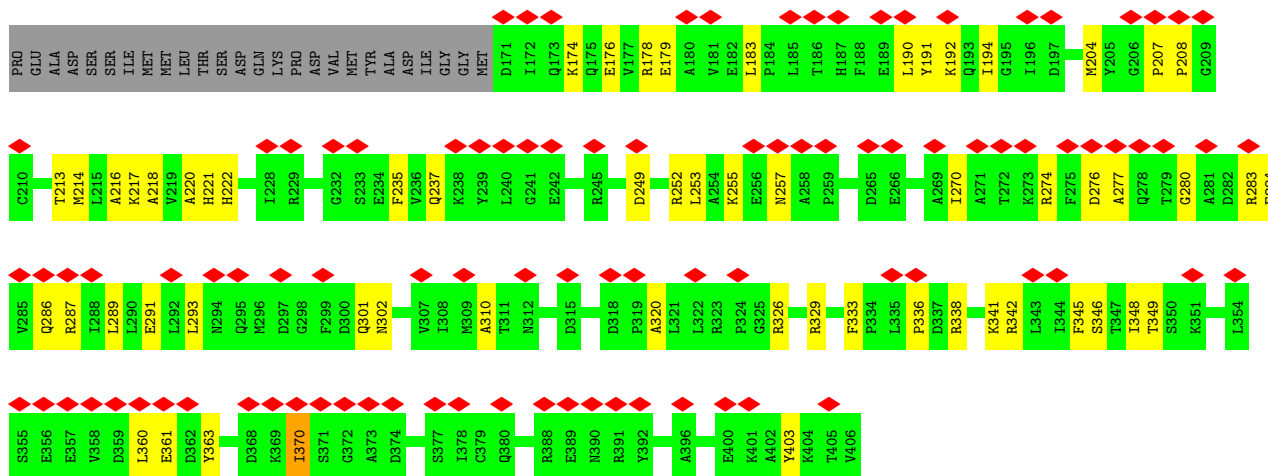


- Molecule 3: 26S proteasome regulatory subunit 4

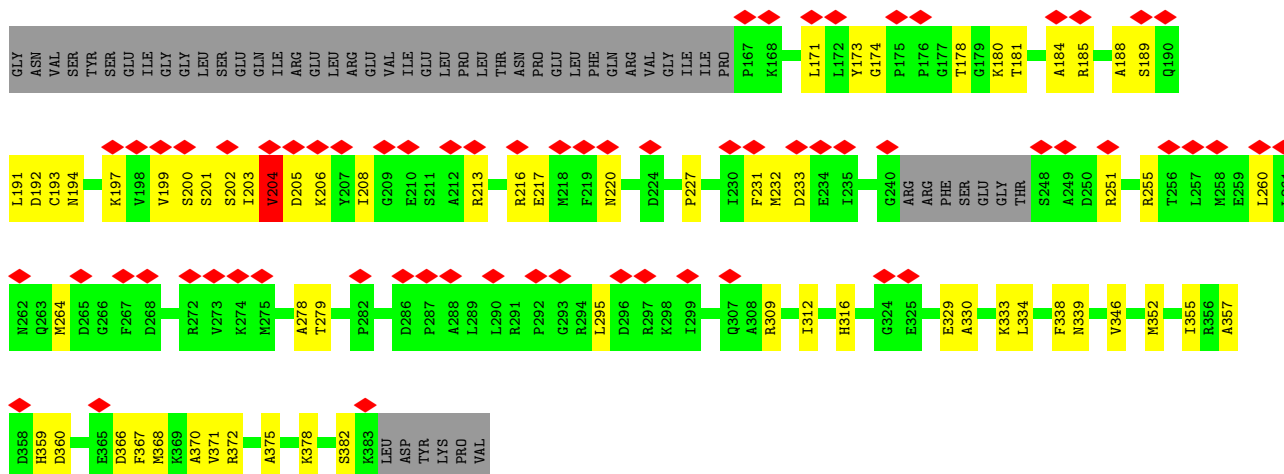




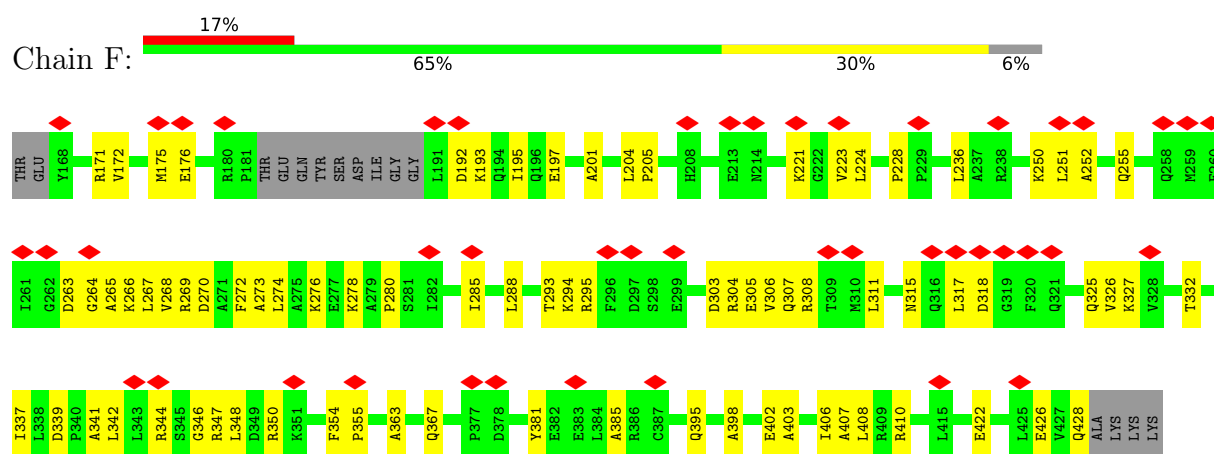
• Molecule 4: 26S proteasome regulatory subunit 6B



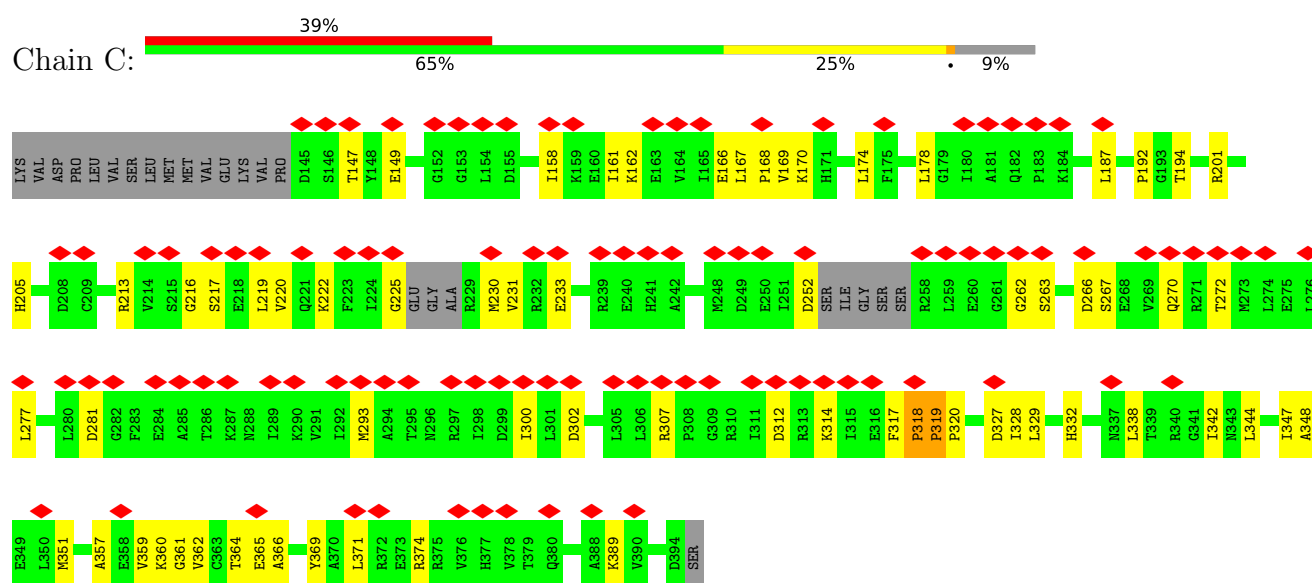
• Molecule 5: 26S proteasome regulatory subunit 10B



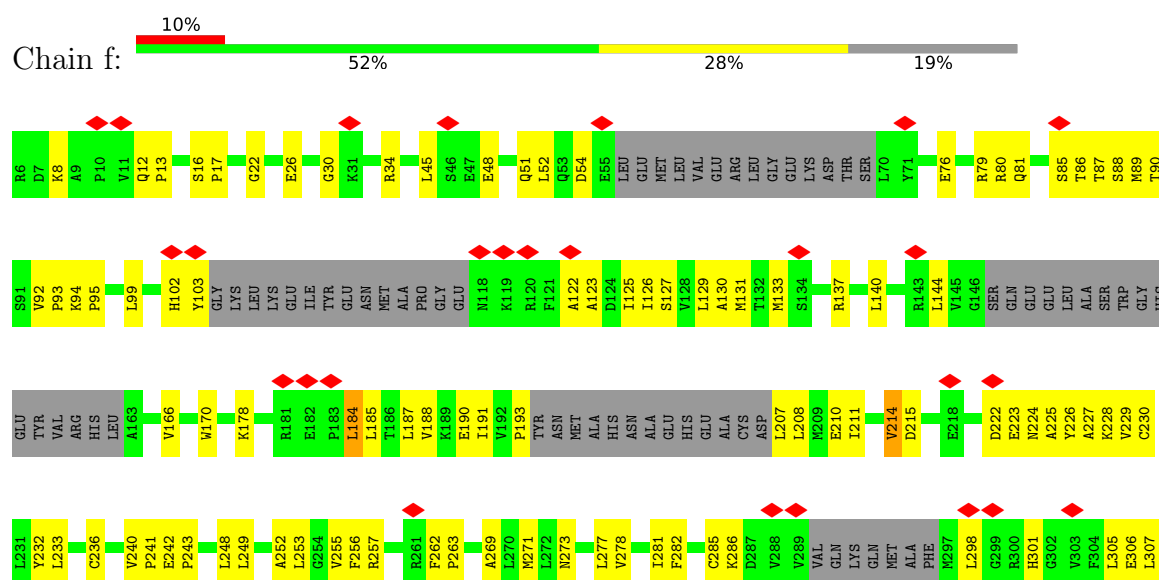
• Molecule 6: 26S proteasome regulatory subunit 6A



• Molecule 7: 26S proteasome regulatory subunit 8



• Molecule 8: 26S proteasome non-ATPase regulatory subunit 2



PRO	ARG	ARG	MET	LEU	VAL	THR	PHE	ASP	GLU	GLU	VAL	ARG	ARG	PRO	PRO	VAL	VAL	SER	VAL	ARG	VAL	VAL	GLY	GLN	ALA	VAL	ASP	VAL	VAL																															
H752	A753	K754	ASP	PRO	ASN	ASN	LEU	PHE	LEU	VAL	VAL	ARG	LEU	LEU	ALA	GLN	GLY	LEU	THR	HIS	LEU	LEU	GLY	K773	L778	C779	P780	Y781	H782	R785	L797	T798	V799	L800	F803	L804	ASP	VAL	ARG	ASN	ASN	ILE	ILE	LEU	GLY	LVS	SER	HIS	THR	VAL	GLY	LEU	THR	GLY	VAL	ALA	ALA	ALA	MET	GLN
G675	G676	H677	L678	L679	P684	R688	A689	V690	L694	A695	V699	SER	ASN	PRO	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	L612	E618	H619	F620	D621	S622	K623	E624	K625	E626	E627	D628	K629	D630	K631	Q632	E633	K634	D638	G647	Q650	G651	V652	A653	V654	L655	G656	I657	A658	L659	I660	A661	H662	A671	T674		
V583	S584	E585	P586	F587	R588	S589	N592	V595	A599	S603	G604	K608	L612	E618	H619	F620	D621	S622	K623	E624	K625	E626	E627	D628	K629	D630	K631	Q632	E633	K634	D638	G647	Q650	G651	V652	A653	V654	L655	G656	I657	A658	L659	I660	A661	H662	A671	T674													
N493	R494	P495	D496	V497	L502	P503	K509	S510	S511	N512	V517	K521	C522	G523	V527	G528	S529	C530	N531	V534	T535	S536	T537	I538	L539	Q540	T541	K545	T541	L463	A464	L465	L466	S467	D468	Y469	V470	L471	H472	N473	S474	M477	R478	L479	G480	S481	I482	Y489	S581	V582										
D310	V311	E312	E313	T314	E315	D316	L317	T318	E319	S322	N323	V324	Q325	L326	N327	S328	N329	F330	L331	A332	L333	A334	R335	E336	L337	D338	I339	E340	P342	D347	K350	T351	H352	L353	E354	N355	N356	R357	F358	G359	G360	S361	G362	S363	Q364	V365	D366	R369	M370	N371	V377									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	G	0.07	0/1540	0.21	0/2084
2	A	0.11	0/2052	0.33	0/2759
3	B	0.10	0/1868	0.29	0/2513
4	D	0.11	0/1903	0.31	0/2568
5	E	0.10	0/1669	0.32	0/2244
6	F	0.10	0/1992	0.28	0/2682
7	C	0.13	0/1915	0.36	0/2570
8	f	0.11	0/5377	0.36	0/7248
All	All	0.11	0/18316	0.32	0/24668

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1516	0	1499	31	0
2	A	2022	0	2079	49	0
3	B	1843	0	1895	29	0
4	D	1873	0	1912	47	0
5	E	1644	0	1667	56	0
6	F	1965	0	2000	63	0
7	C	1890	0	1948	55	0
8	f	5304	0	5315	191	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18057	0	18315	500	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (500) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:301:HIS:O	8:f:305:LEU:HB2	1.52	1.07
8:f:95:PRO:O	8:f:99:LEU:HB2	1.52	1.05
8:f:331:LEU:O	8:f:335:ARG:HB2	1.58	1.04
8:f:324:VAL:O	8:f:325:GLN:HG3	1.60	1.01
8:f:329:ASN:O	8:f:333:LEU:HB2	1.63	0.98
8:f:126:ILE:O	8:f:130:ALA:HB3	1.62	0.97
5:E:216:ARG:O	5:E:220:ASN:HB2	1.64	0.96
7:C:318:PRO:HB2	7:C:319:PRO:HD3	1.46	0.94
8:f:224:ASN:O	8:f:228:LYS:HB3	1.66	0.93
8:f:624:GLU:O	8:f:628:ASP:HB2	1.69	0.92
5:E:330:ALA:O	5:E:334:LEU:HB2	1.69	0.92
8:f:127:SER:O	8:f:131:MET:HB2	1.71	0.90
5:E:367:PHE:O	5:E:371:VAL:HB	1.71	0.90
2:A:161:VAL:O	2:A:165:GLN:HB2	1.70	0.90
8:f:129:LEU:O	8:f:133:MET:HB2	1.74	0.88
8:f:232:TYR:O	8:f:236:CYS:HB2	1.74	0.88
8:f:625:LYS:O	8:f:629:LYS:HB2	1.74	0.88
4:D:174:LYS:O	4:D:178:ARG:HB2	1.74	0.87
8:f:8:LYS:O	8:f:12:GLN:HB2	1.74	0.87
8:f:225:ALA:O	8:f:229:VAL:HB	1.73	0.87
7:C:317:PHE:N	7:C:318:PRO:HD3	1.92	0.85
6:F:274:LEU:O	6:F:278:LYS:HB2	1.77	0.85
8:f:228:LYS:O	8:f:232:TYR:HB3	1.76	0.84
6:F:266:LYS:O	6:F:270:ASP:HB2	1.78	0.84
8:f:318:THR:O	8:f:322:SER:HB3	1.77	0.83
4:D:341:LYS:O	4:D:345:PHE:HB2	1.79	0.83
6:F:272:PHE:O	6:F:276:LYS:HB2	1.79	0.81
8:f:509:LYS:HD3	8:f:511:SER:H	1.45	0.81
8:f:328:SER:O	8:f:332:ALA:HB3	1.82	0.80
1:G:57:GLU:O	1:G:61:GLN:HB2	1.82	0.80
8:f:330:PHE:O	8:f:334:ALA:HB3	1.82	0.78
8:f:236:CYS:HA	8:f:240:VAL:HB	1.66	0.77
2:A:417:ILE:O	2:A:421:ALA:HB3	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:123:ALA:O	8:f:127:SER:HB2	1.83	0.77
3:B:235:LEU:O	3:B:239:VAL:HB	1.84	0.77
8:f:675:PHE:O	8:f:679:LEU:HB2	1.86	0.76
8:f:282:PHE:O	8:f:286:LYS:HB2	1.86	0.75
5:E:366:ASP:O	5:E:370:ALA:HB3	1.86	0.75
7:C:318:PRO:CB	7:C:319:PRO:HD3	2.17	0.74
8:f:301:HIS:O	8:f:305:LEU:CB	2.35	0.74
8:f:229:VAL:O	8:f:233:LEU:HB2	1.89	0.72
8:f:223:GLU:O	8:f:227:ALA:HB3	1.89	0.72
6:F:265:ALA:O	6:F:269:ARG:HB2	1.88	0.72
7:C:361:GLY:O	7:C:365:GLU:HB2	1.89	0.72
2:A:407:LYS:HA	2:A:410:LEU:HD23	1.72	0.71
7:C:317:PHE:N	7:C:318:PRO:CD	2.53	0.71
6:F:263:ASP:O	6:F:267:LEU:HB2	1.91	0.70
7:C:162:LYS:O	7:C:166:GLU:HB2	1.91	0.70
8:f:313:GLU:O	8:f:317:LEU:HB2	1.91	0.70
5:E:213:ARG:O	5:E:217:GLU:HB2	1.92	0.70
8:f:460:ASP:OD1	8:f:460:ASP:N	2.21	0.68
2:A:333:ARG:HH12	2:A:340:LYS:HE2	1.59	0.68
4:D:190:LEU:HD23	7:C:374:ARG:HH21	1.58	0.68
1:G:54:GLU:O	1:G:58:PHE:HB2	1.94	0.68
8:f:359:GLY:O	8:f:363:SER:HB3	1.92	0.68
8:f:749:ALA:O	8:f:753:ALA:HB2	1.94	0.68
8:f:608:LYS:O	8:f:612:LEU:HB2	1.94	0.67
5:E:204:VAL:HG23	5:E:205:ASP:H	1.59	0.67
8:f:80:ARG:HD2	8:f:133:MET:HE1	1.76	0.67
8:f:306:GLU:HB3	8:f:339:ILE:HD12	1.77	0.67
3:B:231:GLY:O	3:B:235:LEU:HB2	1.95	0.67
5:E:368:MET:O	5:E:372:ARG:HB2	1.93	0.67
8:f:269:ALA:HB2	8:f:277:LEU:HD22	1.76	0.67
3:B:194:ILE:O	3:B:198:LYS:HB2	1.95	0.66
2:A:354:ILE:O	2:A:358:HIS:HB2	1.95	0.66
6:F:269:ARG:O	6:F:273:ALA:HB2	1.95	0.66
8:f:341:GLU:HG3	8:f:342:PRO:HD3	1.77	0.66
7:C:216:GLY:HA2	7:C:220:VAL:HG23	1.79	0.65
7:C:317:PHE:H	7:C:318:PRO:HD3	1.62	0.65
4:D:179:GLU:HA	4:D:183:LEU:HD13	1.79	0.65
8:f:129:LEU:O	8:f:133:MET:CB	2.44	0.64
8:f:328:SER:O	8:f:332:ALA:CB	2.45	0.64
7:C:192:PRO:HG2	7:C:357:ALA:HB2	1.80	0.64
5:E:184:ALA:O	5:E:188:ALA:HB3	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:204:LEU:HG	6:F:205:PRO:HD3	1.80	0.64
6:F:221:LYS:HB2	6:F:346:GLY:HA2	1.80	0.64
8:f:618:GLU:HG2	8:f:623:LYS:HD2	1.79	0.64
8:f:369:ARG:HD3	8:f:740:ARG:HB3	1.81	0.63
1:G:157:ILE:HA	1:G:160:TYR:HD2	1.64	0.63
1:G:145:ARG:NH1	4:D:361:GLU:OE1	2.32	0.62
3:B:202:GLU:O	3:B:206:THR:OG1	2.16	0.62
6:F:192:ASP:HA	6:F:195:ILE:HG22	1.81	0.62
2:A:417:ILE:O	2:A:421:ALA:CB	2.47	0.62
5:E:202:SER:HB2	6:F:308:ARG:HD3	1.82	0.62
2:A:208:PRO:HD2	2:A:314:ASN:HD21	1.64	0.62
8:f:517:VAL:O	8:f:521:ALA:HB2	1.99	0.62
8:f:695:ALA:HB1	8:f:753:ALA:HA	1.80	0.62
7:C:158:ILE:HA	7:C:161:ILE:HG22	1.80	0.61
8:f:79:ARG:HH21	8:f:95:PRO:HG3	1.64	0.61
8:f:166:VAL:O	8:f:170:TRP:HB2	2.01	0.61
8:f:399:LEU:HD21	8:f:407:MET:HG3	1.83	0.61
7:C:174:LEU:HB2	7:C:178:LEU:HD13	1.82	0.61
8:f:193:PRO:O	8:f:207:LEU:N	2.34	0.61
8:f:178:LYS:NZ	8:f:215:ASP:O	2.32	0.61
8:f:187:LEU:HA	8:f:190:GLU:HG2	1.83	0.61
3:B:189:GLY:N	3:B:360:THR:HG1	1.99	0.61
8:f:226:TYR:O	8:f:230:CYS:HB2	2.01	0.60
8:f:479:LEU:HA	8:f:517:VAL:HG21	1.82	0.60
5:E:312:ILE:HG13	5:E:316:HIS:HD2	1.66	0.60
4:D:342:ARG:O	4:D:346:SER:HB3	2.00	0.60
6:F:381:TYR:O	6:F:385:ALA:CB	2.50	0.60
8:f:123:ALA:O	8:f:127:SER:CB	2.50	0.60
7:C:329:LEU:HB2	7:C:359:VAL:HG22	1.84	0.60
8:f:253:LEU:O	8:f:257:ARG:HB2	2.01	0.60
2:A:296:GLN:O	2:A:300:LEU:HB2	2.02	0.60
8:f:313:GLU:O	8:f:317:LEU:CB	2.50	0.60
3:B:216:ILE:HG22	3:B:218:PRO:HD3	1.83	0.60
6:F:224:LEU:HD13	6:F:348:LEU:HD13	1.83	0.60
7:C:174:LEU:HD13	7:C:178:LEU:HD22	1.83	0.60
5:E:185:ARG:O	5:E:189:SER:OG	2.20	0.59
8:f:253:LEU:O	8:f:257:ARG:CB	2.50	0.59
7:C:263:SER:O	7:C:267:SER:HB2	2.02	0.59
5:E:368:MET:O	5:E:372:ARG:CB	2.51	0.59
8:f:184:LEU:O	8:f:188:VAL:HB	2.02	0.59
6:F:293:THR:HG22	6:F:295:ARG:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:262:GLY:O	7:C:266:ASP:HB2	2.03	0.59
8:f:89:MET:HG2	8:f:90:THR:HG23	1.84	0.59
8:f:140:LEU:O	8:f:144:LEU:HB2	2.03	0.58
8:f:655:LEU:HB3	8:f:678:LEU:HD11	1.84	0.58
6:F:341:ALA:O	6:F:347:ARG:NH2	2.36	0.58
8:f:229:VAL:O	8:f:233:LEU:CB	2.50	0.58
8:f:586:PRO:HA	8:f:589:SER:HB2	1.83	0.58
4:D:280:GLY:O	4:D:284:GLU:HB2	2.03	0.58
1:G:152:LEU:HD23	1:G:187:GLU:HG2	1.86	0.58
8:f:377:VAL:HG22	8:f:751:TYR:HB2	1.86	0.58
5:E:346:VAL:HG12	5:E:371:VAL:HG22	1.86	0.58
8:f:224:ASN:HB3	8:f:228:LYS:HZ2	1.69	0.58
8:f:347:ASP:O	8:f:351:THR:OG1	2.21	0.57
4:D:283:ARG:HG3	4:D:286:GLN:HE21	1.70	0.57
4:D:342:ARG:O	4:D:346:SER:CB	2.52	0.57
8:f:474:SER:O	8:f:478:ARG:HB2	2.05	0.57
8:f:127:SER:O	8:f:131:MET:CB	2.49	0.57
4:D:218:ALA:O	4:D:222:HIS:ND1	2.36	0.57
5:E:185:ARG:NH2	6:F:318:ASP:O	2.37	0.57
1:G:145:ARG:HG2	4:D:338:ARG:HH22	1.68	0.57
2:A:212:VAL:HA	2:A:339:ARG:HB3	1.87	0.57
8:f:8:LYS:O	8:f:12:GLN:CB	2.50	0.57
8:f:248:LEU:O	8:f:252:ALA:CB	2.52	0.57
8:f:331:LEU:O	8:f:335:ARG:CB	2.45	0.57
6:F:293:THR:HA	6:F:337:ILE:HG21	1.87	0.57
4:D:174:LYS:O	4:D:178:ARG:CB	2.51	0.57
5:E:371:VAL:O	5:E:375:ALA:CB	2.53	0.57
5:E:378:LYS:O	5:E:382:SER:HB3	2.05	0.57
8:f:248:LEU:O	8:f:252:ALA:HB3	2.04	0.57
8:f:307:LEU:HG	8:f:339:ILE:HD11	1.87	0.57
8:f:315:GLU:HA	8:f:318:THR:HG22	1.87	0.57
2:A:200:ARG:O	2:A:204:LEU:HB3	2.05	0.56
1:G:185:VAL:HG12	1:G:189:LYS:HE2	1.86	0.56
2:A:412:ALA:O	2:A:416:VAL:HB	2.05	0.56
6:F:276:LYS:O	6:F:325:GLN:NE2	2.38	0.56
8:f:324:VAL:O	8:f:325:GLN:CG	2.46	0.56
7:C:194:THR:HG21	7:C:359:VAL:HB	1.87	0.56
5:E:178:THR:O	5:E:339:ASN:ND2	2.39	0.56
8:f:654:VAL:HA	8:f:657:ILE:HD12	1.87	0.56
2:A:185:GLU:OE1	2:A:188:ARG:NH2	2.38	0.56
2:A:244:GLU:OE1	2:A:247:GLN:NE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:287:ARG:O	4:D:291:GLU:HB2	2.06	0.56
4:D:320:ALA:O	4:D:326:ARG:NH1	2.39	0.56
4:D:363:TYR:HB3	4:D:403:TYR:HE2	1.70	0.56
5:E:260:LEU:HB3	5:E:264:MET:HE2	1.87	0.56
8:f:536:SER:O	8:f:540:GLN:HB2	2.05	0.56
4:D:287:ARG:HD2	7:C:222:LYS:HB3	1.88	0.56
1:G:9:MET:O	1:G:13:LEU:HB2	2.04	0.56
1:G:135:LYS:HE2	1:G:167:ILE:HG23	1.88	0.56
6:F:318:ASP:OD2	6:F:347:ARG:NH1	2.39	0.56
6:F:342:LEU:HD13	6:F:348:LEU:HD12	1.87	0.56
8:f:466:LEU:O	8:f:478:ARG:NH2	2.37	0.56
3:B:217:LYS:O	3:B:219:PRO:HD3	2.06	0.55
5:E:199:VAL:HG11	6:F:308:ARG:HG3	1.88	0.55
7:C:174:LEU:O	7:C:178:LEU:HB2	2.06	0.55
2:A:271:LEU:HD23	2:A:316:LYS:HD2	1.89	0.55
4:D:192:LYS:HD2	4:D:301:GLN:HE21	1.70	0.55
8:f:226:TYR:O	8:f:230:CYS:CB	2.53	0.55
1:G:78:HIS:O	1:G:82:SER:HB3	2.06	0.55
2:A:312:ARG:HG2	2:A:315:ILE:HG23	1.89	0.55
8:f:253:LEU:HD12	8:f:277:LEU:HD12	1.89	0.55
7:C:147:THR:HG23	7:C:149:GLU:H	1.71	0.55
8:f:122:ALA:O	8:f:126:ILE:HB	2.07	0.55
6:F:363:ALA:O	6:F:367:GLN:HB2	2.06	0.55
2:A:246:VAL:HG13	2:A:280:ILE:HG22	1.88	0.54
7:C:277:LEU:O	7:C:281:ASP:HB2	2.07	0.54
7:C:225:GLY:HA2	7:C:233:GLU:HG3	1.88	0.54
8:f:232:TYR:O	8:f:236:CYS:CB	2.50	0.54
4:D:191:TYR:OH	7:C:374:ARG:NH1	2.41	0.54
4:D:176:GLU:OE2	4:D:329:ARG:NH2	2.41	0.54
8:f:578:ALA:O	8:f:582:VAL:HB	2.08	0.54
5:E:184:ALA:O	5:E:188:ALA:CB	2.55	0.54
8:f:45:LEU:HA	8:f:48:GLU:HG2	1.90	0.54
8:f:282:PHE:O	8:f:286:LYS:CB	2.56	0.54
6:F:280:PRO:HA	6:F:326:VAL:HG22	1.90	0.54
8:f:359:GLY:O	8:f:363:SER:CB	2.55	0.53
5:E:206:LYS:HD2	6:F:305:GLU:HB2	1.89	0.53
6:F:294:LYS:H	6:F:294:LYS:HD2	1.73	0.53
1:G:56:VAL:O	1:G:60:LEU:HB2	2.09	0.53
8:f:30:GLY:O	8:f:34:ARG:HB2	2.08	0.53
8:f:86:THR:HG23	8:f:87:THR:H	1.73	0.53
8:f:553:THR:HA	8:f:556:ARG:HE	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:255:LEU:HD13	3:B:266:LEU:HD22	1.90	0.53
2:A:387:SER:OG	3:B:343:ARG:NH1	2.40	0.53
8:f:477:MET:O	8:f:481:SER:HB2	2.09	0.53
2:A:317:VAL:HB	2:A:337:LEU:HG	1.90	0.53
4:D:283:ARG:HA	4:D:286:GLN:HG2	1.91	0.53
5:E:188:ALA:HB2	5:E:231:PHE:HE2	1.74	0.53
5:E:329:GLU:O	5:E:333:LYS:HB3	2.09	0.53
1:G:37:ASP:OD2	1:G:41:ARG:NH2	2.39	0.53
2:A:200:ARG:O	2:A:204:LEU:CB	2.57	0.53
5:E:185:ARG:O	5:E:189:SER:CB	2.56	0.53
6:F:422:GLU:O	6:F:426:GLU:HB2	2.09	0.53
7:C:270:GLN:NE2	7:C:302:ASP:OD2	2.42	0.53
2:A:414:ASN:O	2:A:418:LYS:HB3	2.09	0.53
5:E:371:VAL:O	5:E:375:ALA:HB2	2.08	0.53
7:C:307:ARG:NH2	7:C:312:ASP:OD2	2.42	0.53
7:C:263:SER:O	7:C:267:SER:CB	2.57	0.53
5:E:233:ASP:HA	5:E:278:ALA:HB3	1.90	0.52
6:F:398:ALA:O	6:F:402:GLU:HB2	2.09	0.52
8:f:350:LYS:HG3	8:f:351:THR:HG23	1.90	0.52
8:f:416:MET:HG2	8:f:450:ILE:HG21	1.91	0.52
2:A:391:GLU:HA	2:A:394:MET:HB3	1.92	0.52
4:D:346:SER:HA	4:D:349:THR:HG22	1.89	0.52
5:E:174:GLY:H	5:E:180:LYS:HZ1	1.57	0.52
8:f:403:LYS:HG2	8:f:404:ASP:H	1.73	0.52
3:B:333:ARG:HG2	3:B:335:GLU:H	1.75	0.52
8:f:228:LYS:O	8:f:232:TYR:CB	2.54	0.52
7:C:362:VAL:O	7:C:366:ALA:CB	2.57	0.52
8:f:208:LEU:HG	8:f:210:GLU:HB2	1.92	0.52
6:F:264:GLY:O	6:F:268:VAL:HB	2.09	0.52
7:C:318:PRO:HB2	7:C:319:PRO:CD	2.27	0.52
5:E:200:SER:OG	5:E:233:ASP:O	2.27	0.52
5:E:309:ARG:HH22	5:E:338:PHE:H	1.56	0.52
2:A:191:VAL:HG13	2:A:192:GLU:HG3	1.90	0.52
8:f:512:MET:HE2	8:f:557:TRP:HB2	1.91	0.52
8:f:52:LEU:HD12	8:f:79:ARG:HD2	1.91	0.52
5:E:199:VAL:HG12	5:E:201:SER:H	1.74	0.51
6:F:266:LYS:O	6:F:270:ASP:CB	2.53	0.51
8:f:80:ARG:HB3	8:f:95:PRO:HB2	1.92	0.51
1:G:90:LYS:HE2	1:G:124:MET:HE1	1.92	0.51
6:F:293:THR:O	6:F:307:GLN:NE2	2.41	0.51
8:f:22:GLY:O	8:f:26:GLU:HB2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:398:ALA:O	6:F:402:GLU:CB	2.59	0.51
6:F:325:GLN:HG2	6:F:326:VAL:H	1.76	0.51
5:E:352:MET:SD	6:F:350:ARG:NH1	2.84	0.51
8:f:446:LEU:HD21	8:f:799:VAL:HG11	1.93	0.51
5:E:213:ARG:O	5:E:217:GLU:CB	2.59	0.51
4:D:270:ILE:HG13	4:D:289:LEU:HD22	1.93	0.51
6:F:176:GLU:HG3	6:F:250:LYS:HB2	1.93	0.50
5:E:357:ALA:O	5:E:359:HIS:ND1	2.45	0.50
5:E:309:ARG:HH12	5:E:338:PHE:HB2	1.76	0.50
6:F:268:VAL:O	6:F:272:PHE:HB2	2.11	0.50
8:f:477:MET:O	8:f:481:SER:CB	2.60	0.50
8:f:187:LEU:HD13	8:f:228:LYS:HB2	1.92	0.50
8:f:140:LEU:O	8:f:144:LEU:CB	2.60	0.50
8:f:660:ILE:HG21	8:f:785:ARG:HD2	1.93	0.50
7:C:167:LEU:HD21	7:C:174:LEU:HD11	1.92	0.50
7:C:167:LEU:HB3	7:C:168:PRO:HD3	1.94	0.50
1:G:114:ALA:HA	1:G:154:MET:HE3	1.92	0.49
2:A:415:LYS:O	2:A:419:SER:OG	2.30	0.49
5:E:180:LYS:NZ	5:E:279:THR:O	2.29	0.49
6:F:171:ARG:HG3	6:F:172:VAL:HG23	1.93	0.49
8:f:325:GLN:HG2	8:f:331:LEU:HG	1.94	0.49
6:F:251:LEU:HB3	6:F:285:ILE:HG22	1.94	0.49
8:f:278:VAL:HA	8:f:281:ILE:HG22	1.93	0.49
6:F:381:TYR:O	6:F:385:ALA:HB2	2.11	0.49
7:C:262:GLY:O	7:C:266:ASP:CB	2.60	0.49
8:f:695:ALA:HB3	8:f:752:HIS:CE1	2.47	0.49
8:f:190:GLU:C	8:f:193:PRO:HD2	2.38	0.49
4:D:274:ARG:NH1	4:D:276:ASP:OD2	2.44	0.49
7:C:328:ILE:O	7:C:332:HIS:ND1	2.35	0.49
3:B:194:ILE:O	3:B:198:LYS:CB	2.60	0.49
7:C:317:PHE:CE1	7:C:320:PRO:HB3	2.48	0.49
8:f:366:ASP:H	8:f:370:MET:HB2	1.78	0.49
8:f:545:LYS:HE2	8:f:555:ALA:HA	1.95	0.49
1:G:72:ALA:HB1	1:G:104:GLN:HB2	1.94	0.49
1:G:147:ALA:HB1	1:G:179:ALA:HB2	1.95	0.49
4:D:277:ALA:HB2	7:C:230:MET:HG2	1.94	0.49
7:C:344:LEU:O	7:C:348:ALA:CB	2.61	0.49
4:D:216:ALA:O	4:D:220:ALA:CB	2.61	0.49
8:f:316:ASP:O	8:f:319:GLU:HG2	2.13	0.49
4:D:214:MET:O	4:D:218:ALA:HB2	2.12	0.48
6:F:317:LEU:O	6:F:344:ARG:NH1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:12:GLN:HB3	8:f:13:PRO:HD3	1.95	0.48
8:f:125:ILE:HA	8:f:129:LEU:HD12	1.95	0.48
8:f:325:GLN:CD	8:f:328:SER:H	2.20	0.48
1:G:180:CYS:HB3	1:G:212:ALA:HB2	1.95	0.48
5:E:180:LYS:HD3	5:E:278:ALA:HB1	1.95	0.48
8:f:51:GLN:HA	8:f:54:ASP:HB2	1.95	0.48
8:f:624:GLU:O	8:f:628:ASP:CB	2.53	0.48
6:F:223:VAL:HG23	6:F:350:ARG:HB2	1.94	0.48
6:F:193:LYS:HD2	6:F:355:PRO:HG3	1.94	0.48
2:A:258:ARG:O	2:A:262:GLU:HB2	2.13	0.48
8:f:418:LEU:HD13	8:f:425:GLY:HA2	1.95	0.48
8:f:517:VAL:O	8:f:521:ALA:CB	2.62	0.48
1:G:11:CYS:O	1:G:15:TYR:HB2	2.14	0.48
2:A:188:ARG:HA	2:A:191:VAL:HG12	1.96	0.48
8:f:569:LYS:HE3	8:f:599:ALA:HA	1.96	0.48
8:f:224:ASN:O	8:f:228:LYS:CB	2.53	0.48
2:A:184:ILE:O	2:A:188:ARG:HB2	2.14	0.48
4:D:207:PRO:HG2	4:D:208:PRO:HD3	1.96	0.48
5:E:312:ILE:HG13	5:E:316:HIS:CD2	2.47	0.48
6:F:288:LEU:HB3	6:F:332:THR:HG22	1.95	0.48
8:f:798:THR:HG23	8:f:799:VAL:HG13	1.96	0.48
2:A:420:TYR:OH	3:B:346:ARG:NH1	2.47	0.48
5:E:232:MET:O	5:E:278:ALA:N	2.46	0.47
8:f:249:LEU:HD21	8:f:271:MET:HG3	1.96	0.47
3:B:357:ASP:O	3:B:358:GLU:HG3	2.14	0.47
4:D:333:PHE:CZ	4:D:336:PRO:HG3	2.49	0.47
7:C:213:ARG:HH11	7:C:217:SER:HB3	1.79	0.47
8:f:76:GLU:OE1	8:f:79:ARG:NH2	2.47	0.47
8:f:538:ILE:HA	8:f:541:THR:HG22	1.95	0.47
3:B:220:LYS:NZ	3:B:317:ASP:O	2.47	0.47
1:G:60:LEU:HD13	1:G:95:LYS:HG3	1.96	0.47
2:A:401:ARG:NH1	2:A:403:ILE:O	2.48	0.47
5:E:203:ILE:HB	6:F:304:ARG:HH12	1.79	0.47
8:f:273:ASN:ND2	8:f:310:ASP:OD2	2.48	0.47
8:f:632:LYS:HB3	8:f:661:ALA:HA	1.96	0.47
1:G:78:HIS:O	1:G:82:SER:CB	2.63	0.47
4:D:253:LEU:O	4:D:257:ASN:HB3	2.14	0.47
4:D:287:ARG:HH11	7:C:222:LYS:HE3	1.78	0.47
7:C:318:PRO:CB	7:C:319:PRO:CD	2.89	0.47
8:f:474:SER:HA	8:f:477:MET:HB3	1.96	0.47
8:f:531:ASN:HA	8:f:569:LYS:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:213:ARG:HD2	7:C:217:SER:H	1.80	0.47
8:f:92:VAL:O	8:f:95:PRO:HD2	2.14	0.47
8:f:94:LYS:HB3	8:f:95:PRO:HD3	1.96	0.47
8:f:466:LEU:HA	8:f:474:SER:HB3	1.97	0.47
2:A:232:ARG:HH22	2:A:271:LEU:HD13	1.80	0.47
8:f:325:GLN:OE1	8:f:328:SER:N	2.45	0.47
3:B:398:ILE:HA	3:B:401:GLU:HG2	1.97	0.46
8:f:229:VAL:HG21	8:f:256:PHE:CZ	2.50	0.46
2:A:174:TYR:HA	2:A:227:ARG:HD3	1.98	0.46
2:A:414:ASN:O	2:A:418:LYS:CB	2.63	0.46
4:D:204:MET:HE3	4:D:310:ALA:HB2	1.96	0.46
6:F:228:PRO:HD2	6:F:354:PHE:HB2	1.97	0.46
8:f:22:GLY:O	8:f:26:GLU:CB	2.63	0.46
8:f:358:PHE:HZ	8:f:381:VAL:HG21	1.79	0.46
8:f:630:ASP:HB3	8:f:634:LYS:HE3	1.98	0.46
1:G:75:SER:OG	1:G:78:HIS:ND1	2.45	0.46
6:F:197:GLU:O	6:F:201:ALA:CB	2.64	0.46
6:F:252:ALA:HB3	6:F:255:GLN:HG2	1.98	0.46
7:C:362:VAL:O	7:C:366:ALA:HB2	2.15	0.46
8:f:470:VAL:HG13	8:f:471:LEU:H	1.80	0.46
6:F:221:LYS:HZ3	6:F:327:LYS:HE3	1.81	0.46
6:F:269:ARG:O	6:F:273:ALA:CB	2.61	0.46
6:F:272:PHE:O	6:F:276:LYS:CB	2.55	0.46
6:F:381:TYR:O	6:F:385:ALA:HB3	2.15	0.46
8:f:324:VAL:C	8:f:325:GLN:HG3	2.38	0.46
8:f:536:SER:HA	8:f:539:LEU:HB3	1.97	0.46
1:G:11:CYS:O	1:G:15:TYR:CB	2.63	0.46
2:A:411:GLU:O	2:A:415:LYS:CB	2.63	0.46
3:B:201:VAL:HG21	3:B:241:ASN:HD21	1.79	0.46
8:f:102:HIS:CG	8:f:103:TYR:H	2.34	0.46
3:B:270:LEU:HA	3:B:273:VAL:HG12	1.97	0.46
8:f:298:LEU:HA	8:f:301:HIS:CD2	2.50	0.46
8:f:684:PRO:O	8:f:688:ARG:CB	2.64	0.46
1:G:9:MET:O	1:G:13:LEU:CB	2.64	0.46
2:A:354:ILE:HG21	2:A:385:ILE:HD12	1.98	0.46
4:D:360:LEU:HA	4:D:363:TYR:HB2	1.98	0.46
8:f:631:LYS:HA	8:f:634:LYS:HZ2	1.81	0.46
2:A:270:CYS:SG	2:A:271:LEU:N	2.89	0.45
8:f:166:VAL:O	8:f:170:TRP:CB	2.63	0.45
6:F:175:MET:HG3	6:F:176:GLU:H	1.80	0.45
8:f:502:LEU:HB3	8:f:503:PRO:HD3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:315:ILE:HG13	2:A:316:LYS:H	1.81	0.45
8:f:252:ALA:HA	8:f:255:VAL:HG22	1.98	0.45
2:A:190:VAL:HG23	2:A:209:PRO:HG2	1.98	0.45
5:E:203:ILE:H	6:F:304:ARG:HH12	1.62	0.45
8:f:222:ASP:O	8:f:226:TYR:HB3	2.16	0.45
8:f:241:PRO:HB2	8:f:243:PRO:HD2	1.98	0.45
8:f:281:ILE:O	8:f:285:CYS:CB	2.64	0.45
3:B:231:GLY:O	3:B:235:LEU:CB	2.63	0.45
3:B:395:ILE:HA	3:B:398:ILE:HG12	1.98	0.45
5:E:197:LYS:HG2	6:F:315:ASN:ND2	2.32	0.45
6:F:197:GLU:OE2	6:F:350:ARG:NH2	2.49	0.45
8:f:780:PRO:HB3	8:f:800:LEU:HD22	1.97	0.45
1:G:54:GLU:O	1:G:58:PHE:CB	2.64	0.45
4:D:252:ARG:HA	4:D:255:LYS:HG2	1.98	0.45
8:f:573:ILE:HG22	8:f:576:ILE:HB	1.98	0.45
8:f:742:ALA:O	8:f:746:ARG:HB3	2.16	0.45
1:G:131:ASN:HB3	1:G:134:ALA:HB2	1.99	0.45
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.99	0.45
8:f:242:GLU:N	8:f:243:PRO:HD2	2.32	0.45
8:f:325:GLN:NE2	8:f:328:SER:H	2.14	0.45
3:B:223:ILE:HG12	3:B:329:MET:HB2	1.99	0.45
4:D:253:LEU:O	4:D:257:ASN:CB	2.65	0.45
7:C:327:ASP:OD1	7:C:328:ILE:N	2.49	0.45
2:A:165:GLN:HE22	2:A:260:LEU:HB2	1.82	0.44
2:A:351:ARG:HA	2:A:354:ILE:HD13	1.97	0.44
8:f:185:LEU:HA	8:f:188:VAL:HG12	1.98	0.44
8:f:325:GLN:HE22	8:f:328:SER:H	1.65	0.44
8:f:684:PRO:O	8:f:688:ARG:HB2	2.17	0.44
2:A:229:VAL:HG13	2:A:236:CYS:HB2	1.99	0.44
2:A:277:ILE:HG22	2:A:321:THR:HB	1.99	0.44
7:C:231:VAL:HG12	7:C:272:THR:HG23	1.99	0.44
7:C:360:LYS:O	7:C:364:THR:OG1	2.33	0.44
8:f:595:VAL:O	8:f:599:ALA:HB2	2.18	0.44
8:f:671:ALA:O	8:f:674:THR:OG1	2.24	0.44
4:D:249:ASP:HA	4:D:252:ARG:HG2	1.98	0.44
4:D:191:TYR:HE1	7:C:371:LEU:HG	1.81	0.44
5:E:191:LEU:C	5:E:193:CYS:H	2.26	0.44
5:E:194:ASN:HD21	5:E:227:PRO:HG2	1.83	0.44
8:f:620:PHE:CE2	8:f:622:SER:HB3	2.53	0.44
3:B:192:ASN:HA	3:B:195:GLN:HG2	1.99	0.44
5:E:173:TYR:HA	5:E:180:LYS:HZ3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:344:LEU:O	7:C:348:ALA:HB3	2.18	0.43
8:f:93:PRO:HB2	8:f:137:ARG:HE	1.83	0.43
8:f:232:TYR:CE2	8:f:248:LEU:HD12	2.52	0.43
7:C:169:VAL:HG12	7:C:170:LYS:HG3	1.99	0.43
8:f:325:GLN:HB2	8:f:330:PHE:HB2	2.00	0.43
7:C:338:LEU:HD11	7:C:342:ILE:HG21	2.00	0.43
8:f:675:PHE:CG	8:f:694:LEU:HD23	2.54	0.43
6:F:195:ILE:HD12	6:F:236:LEU:HD11	2.01	0.43
1:G:148:ALA:HB2	1:G:178:LEU:HB3	2.00	0.43
5:E:197:LYS:HG2	6:F:315:ASN:HD21	1.83	0.43
5:E:366:ASP:O	5:E:370:ALA:CB	2.59	0.43
2:A:411:GLU:O	2:A:415:LYS:HB3	2.18	0.43
3:B:387:LYS:HD2	3:B:390:LEU:HD22	2.01	0.43
8:f:496:ASP:OD1	8:f:497:VAL:N	2.50	0.43
2:A:395:PHE:HD1	2:A:398:ARG:HD3	1.84	0.43
4:D:217:LYS:O	4:D:221:HIS:HB2	2.19	0.43
2:A:384:GLU:HG3	3:B:343:ARG:HH12	1.84	0.42
8:f:652:VAL:HA	8:f:655:LEU:HD13	2.01	0.42
8:f:658:ALA:HA	8:f:661:ALA:HB3	2.00	0.42
2:A:365:GLU:HG2	2:A:367:ASP:H	1.83	0.42
2:A:418:LYS:O	2:A:422:LYS:HG3	2.19	0.42
8:f:102:HIS:CD2	8:f:103:TYR:H	2.36	0.42
8:f:357:ARG:O	8:f:361:SER:HB2	2.19	0.42
8:f:358:PHE:O	8:f:362:GLY:HA3	2.18	0.42
5:E:185:ARG:O	5:E:189:SER:HB3	2.19	0.42
4:D:191:TYR:HB2	4:D:302:ASN:HD21	1.85	0.42
7:C:369:TYR:HE2	7:C:389:LYS:HG3	1.84	0.42
8:f:327:ASN:C	8:f:329:ASN:H	2.28	0.42
5:E:251:ARG:HH11	5:E:255:ARG:HH21	1.68	0.42
8:f:191:ILE:HD12	8:f:232:TYR:CD1	2.55	0.42
8:f:523:GLY:O	8:f:527:VAL:HG13	2.19	0.42
1:G:147:ALA:HA	1:G:155:ILE:HD11	2.01	0.42
5:E:360:ASP:N	5:E:360:ASP:OD1	2.51	0.42
7:C:187:LEU:HD11	7:C:314:LYS:HE2	2.01	0.42
8:f:229:VAL:HG21	8:f:256:PHE:HZ	1.84	0.42
8:f:262:PHE:HB3	8:f:281:ILE:HD11	2.01	0.42
8:f:584:SER:OG	8:f:588:ARG:HB2	2.19	0.42
2:A:201:PHE:HA	6:F:408:LEU:HD11	2.01	0.42
4:D:213:THR:O	4:D:217:LYS:HB2	2.20	0.42
5:E:329:GLU:O	5:E:333:LYS:CB	2.67	0.42
4:D:191:TYR:HA	4:D:194:ILE:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:281:ILE:O	8:f:285:CYS:HB3	2.19	0.42
8:f:748:LEU:HD23	8:f:752:HIS:CD2	2.54	0.42
4:D:336:PRO:HG2	4:D:341:LYS:HE2	2.02	0.42
4:D:345:PHE:HA	4:D:348:ILE:HG22	2.01	0.41
8:f:438:ASP:OD1	8:f:438:ASP:N	2.52	0.41
8:f:638:ASP:N	8:f:638:ASP:OD1	2.49	0.41
4:D:293:LEU:HD11	4:D:326:ARG:HG2	2.02	0.41
5:E:352:MET:HA	5:E:355:ILE:HG22	2.02	0.41
8:f:262:PHE:N	8:f:263:PRO:HD2	2.35	0.41
8:f:330:PHE:O	8:f:334:ALA:CB	2.61	0.41
8:f:625:LYS:O	8:f:629:LYS:CB	2.56	0.41
8:f:778:LEU:HA	8:f:781:TYR:HE1	1.84	0.41
1:G:70:ASP:OD1	1:G:74:TRP:N	2.53	0.41
2:A:394:MET:HE3	2:A:398:ARG:HD2	2.02	0.41
4:D:342:ARG:O	4:D:346:SER:OG	2.36	0.41
8:f:126:ILE:O	8:f:130:ALA:CB	2.50	0.41
5:E:192:ASP:C	5:E:194:ASN:H	2.27	0.41
5:E:208:ILE:HD12	5:E:208:ILE:H	1.84	0.41
6:F:406:ILE:O	6:F:410:ARG:HG3	2.20	0.41
2:A:372:LEU:HD12	2:A:375:ARG:HE	1.86	0.41
3:B:401:GLU:HG3	3:B:422:SER:HB2	2.02	0.41
8:f:16:SER:HB3	8:f:17:PRO:HD3	2.02	0.41
8:f:371:ASN:OD1	8:f:398:TRP:NE1	2.54	0.41
6:F:311:LEU:O	6:F:315:ASN:HB2	2.21	0.41
1:G:77:LEU:HD23	1:G:109:PRO:HG2	2.03	0.41
7:C:252:ASP:HA	7:C:300:ILE:HD11	2.03	0.41
8:f:81:GLN:O	8:f:85:SER:HB2	2.20	0.41
8:f:211:ILE:O	8:f:214:VAL:HG22	2.21	0.41
2:A:166:VAL:HA	2:A:238:ILE:HD12	2.03	0.41
3:B:380:LEU:O	3:B:384:ILE:HG12	2.21	0.41
3:B:390:LEU:HD23	3:B:394:ASP:HB3	2.03	0.41
4:D:370:ILE:H	4:D:370:ILE:HG13	1.64	0.41
3:B:304:GLU:HA	3:B:307:ARG:HG2	2.03	0.41
5:E:367:PHE:O	5:E:371:VAL:CB	2.58	0.41
6:F:172:VAL:HG11	6:F:267:LEU:HG	2.02	0.41
6:F:303:ASP:OD1	6:F:306:VAL:HB	2.21	0.41
6:F:339:ASP:HB3	6:F:342:LEU:HG	2.03	0.41
7:C:348:ALA:HA	7:C:351:MET:HE2	2.03	0.41
8:f:675:PHE:HD1	8:f:690:VAL:HG23	1.86	0.41
1:G:141:THR:H	1:G:144:HIS:HD2	1.68	0.41
4:D:235:PHE:HA	4:D:237:GLN:HE22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:373:THR:OG1	3:B:412:MET:O	2.39	0.40
6:F:395:GLN:HB3	6:F:428:GLN:NE2	2.36	0.40
7:C:277:LEU:O	7:C:281:ASP:CB	2.69	0.40
8:f:88:SER:HB2	8:f:92:VAL:HG23	2.02	0.40
8:f:337:LEU:O	8:f:341:GLU:HB3	2.21	0.40
8:f:743:ALA:HA	8:f:746:ARG:HG2	2.03	0.40
1:G:177:HIS:CE1	1:G:208:PRO:HG3	2.56	0.40
3:B:191:ASP:HA	3:B:194:ILE:HG22	2.03	0.40
6:F:403:ALA:O	6:F:407:ALA:CB	2.69	0.40
8:f:478:ARG:O	8:f:482:ILE:HB	2.20	0.40
7:C:187:LEU:HB3	7:C:293:MET:HB2	2.03	0.40
7:C:201:ARG:O	7:C:205:HIS:HB2	2.22	0.40
4:D:214:MET:O	4:D:218:ALA:CB	2.68	0.40
5:E:181:THR:O	5:E:185:ARG:HB2	2.22	0.40
7:C:344:LEU:HA	7:C:347:ILE:HG22	2.02	0.40
8:f:579:ALA:HA	8:f:592:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	195/223 (87%)	191 (98%)	4 (2%)	0	100	100
2	A	254/266 (96%)	230 (91%)	24 (9%)	0	100	100
3	B	229/267 (86%)	216 (94%)	13 (6%)	0	100	100
4	D	234/262 (89%)	224 (96%)	10 (4%)	0	100	100
5	E	206/262 (79%)	185 (90%)	20 (10%)	1 (0%)	24	63
6	F	248/267 (93%)	233 (94%)	15 (6%)	0	100	100
7	C	236/266 (89%)	222 (94%)	12 (5%)	2 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	f	664/848 (78%)	598 (90%)	66 (10%)	0	100	100
All	All	2266/2661 (85%)	2099 (93%)	164 (7%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	318	PRO
7	C	319	PRO
5	E	204	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	159/178 (89%)	157 (99%)	2 (1%)	61	74
2	A	219/224 (98%)	217 (99%)	2 (1%)	70	79
3	B	203/231 (88%)	202 (100%)	1 (0%)	81	83
4	D	202/224 (90%)	201 (100%)	1 (0%)	81	83
5	E	178/225 (79%)	177 (99%)	1 (1%)	78	83
6	F	210/222 (95%)	210 (100%)	0	100	100
7	C	204/225 (91%)	203 (100%)	1 (0%)	81	83
8	f	579/714 (81%)	572 (99%)	7 (1%)	63	75
All	All	1954/2243 (87%)	1939 (99%)	15 (1%)	70	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	26	ILE
1	G	55	ILE
2	A	222	LYS
2	A	416	VAL
3	B	260	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	370	ILE
5	E	204	VAL
7	C	219	LEU
8	f	184	LEU
8	f	214	VAL
8	f	364	GLN
8	f	391	LEU
8	f	460	ASP
8	f	470	VAL
8	f	745	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	38	GLN
1	G	98	GLN
1	G	117	ASN
1	G	137	HIS
1	G	166	ASN
2	A	165	GLN
2	A	314	ASN
2	A	353	HIS
4	D	221	HIS
4	D	237	GLN
4	D	301	GLN
5	E	194	ASN
5	E	262	ASN
5	E	307	GLN
5	E	316	HIS
5	E	345	ASN
6	F	258	GLN
6	F	315	ASN
6	F	323	ASN
6	F	367	GLN
7	C	270	GLN
8	f	81	GLN
8	f	102	HIS
8	f	273	ASN
8	f	327	ASN
8	f	475	ASN
8	f	493	ASN
8	f	649	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	f	747	GLN
8	f	752	HIS
8	f	790	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

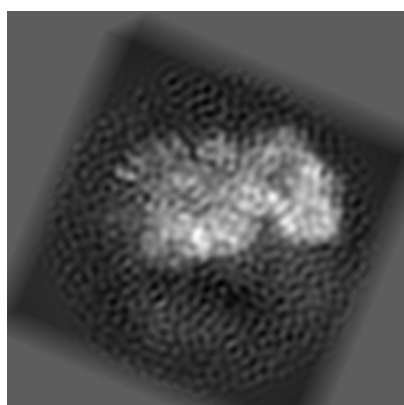
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8683. These allow visual inspection of the internal detail of the map and identification of artifacts.

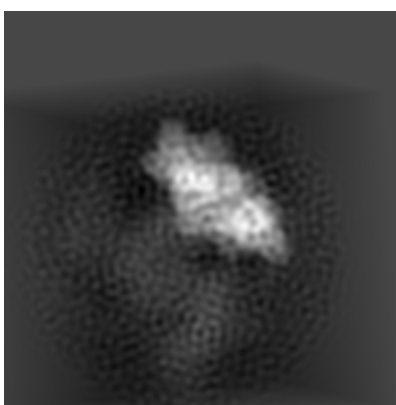
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

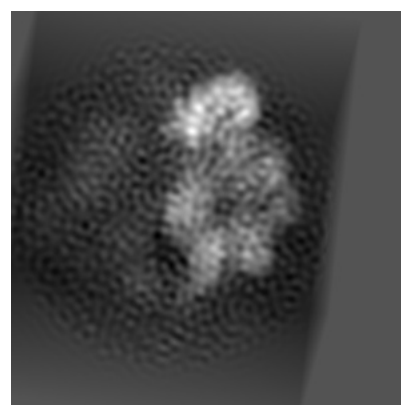
6.1.1 Primary map



X



Y

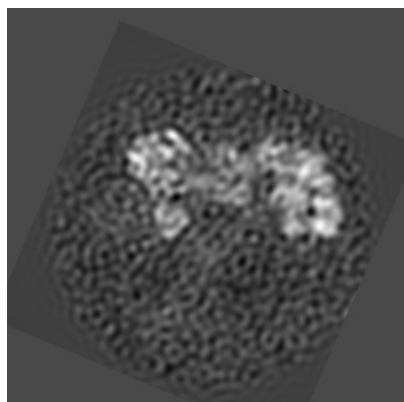


Z

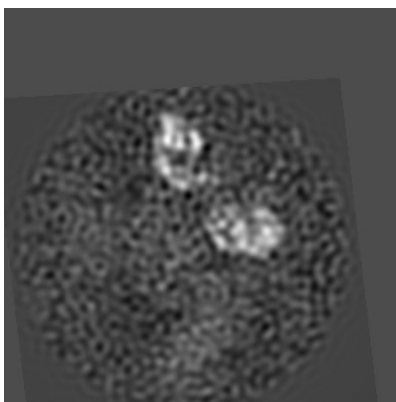
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

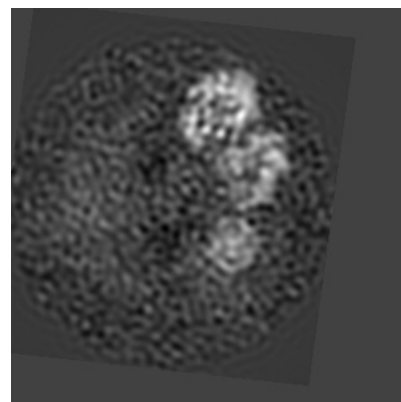
6.2.1 Primary map



X Index: 180



Y Index: 180

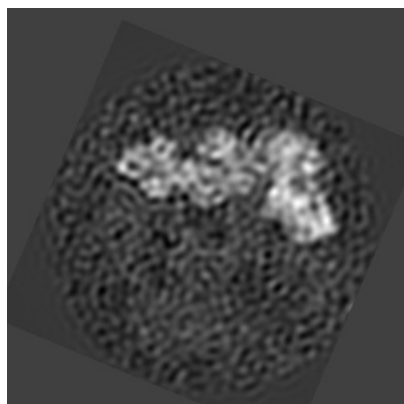


Z Index: 180

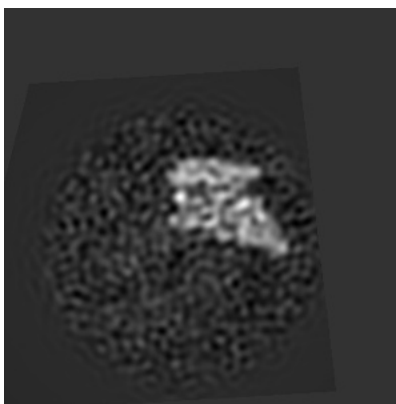
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

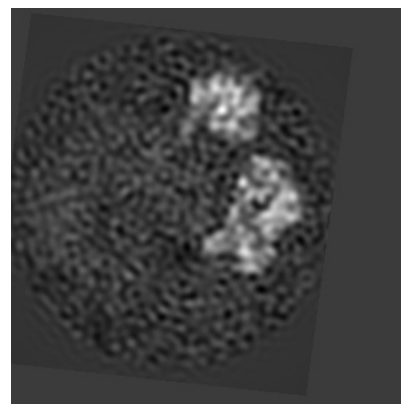
6.3.1 Primary map



X Index: 165



Y Index: 267

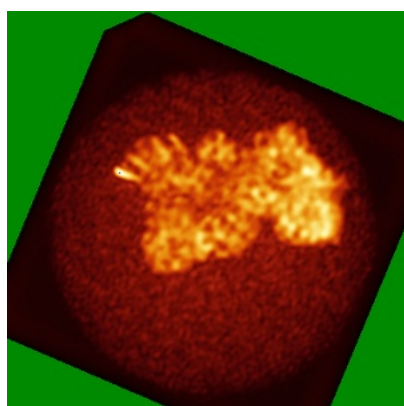


Z Index: 158

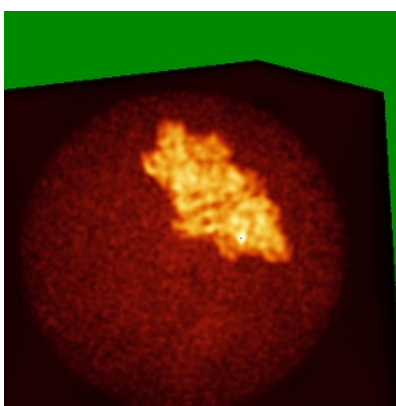
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

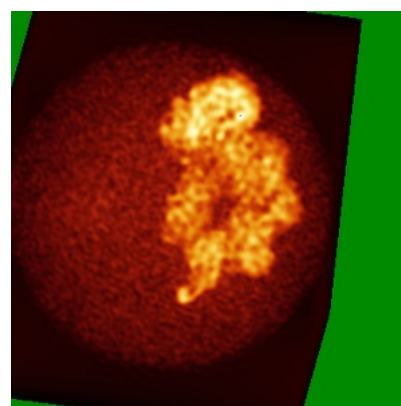
6.4.1 Primary map



X



Y

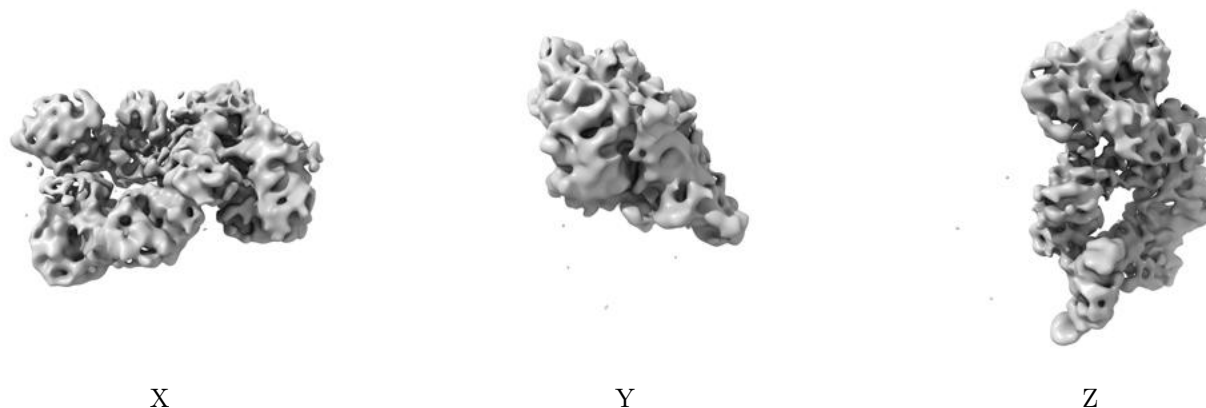


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

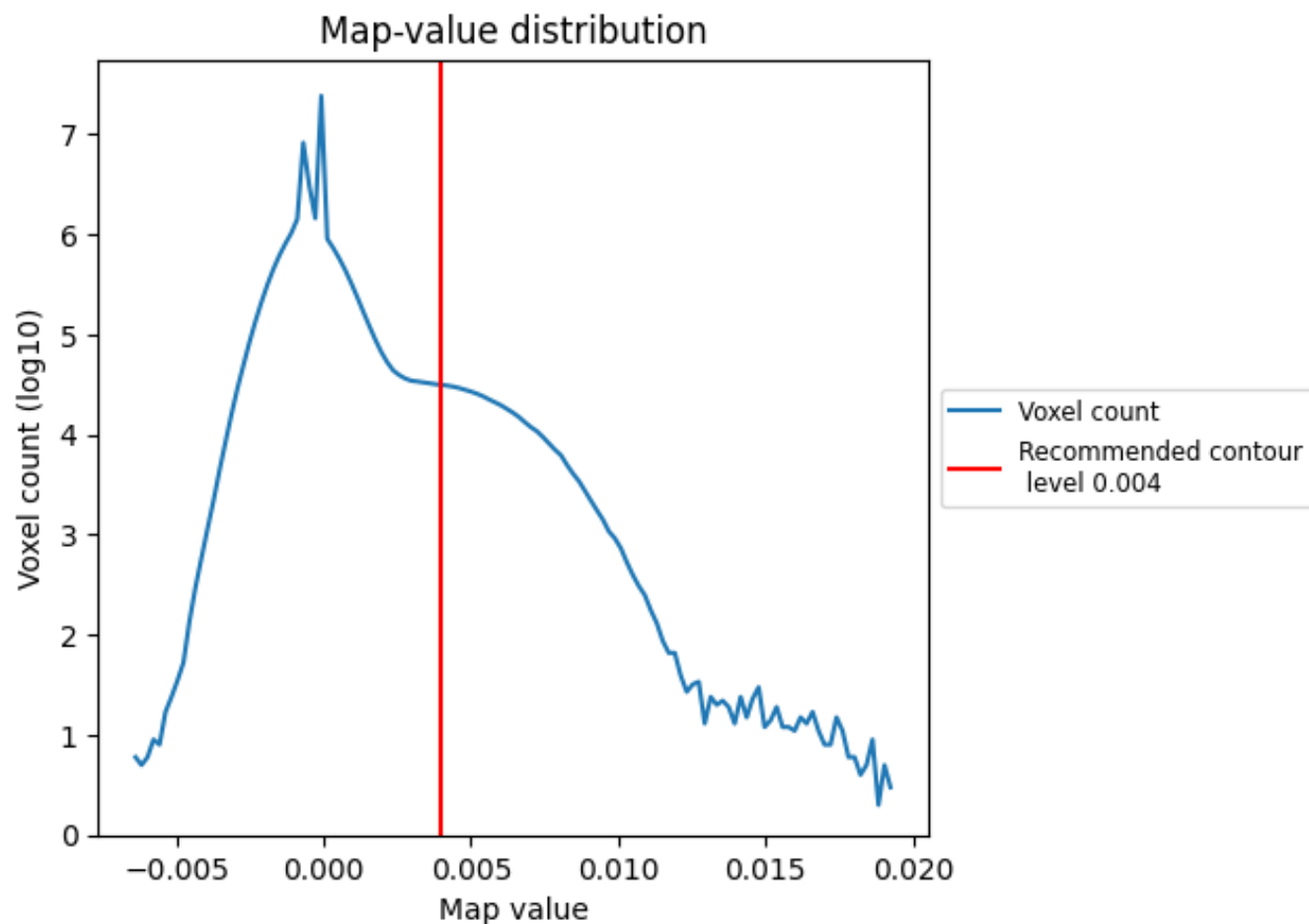
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

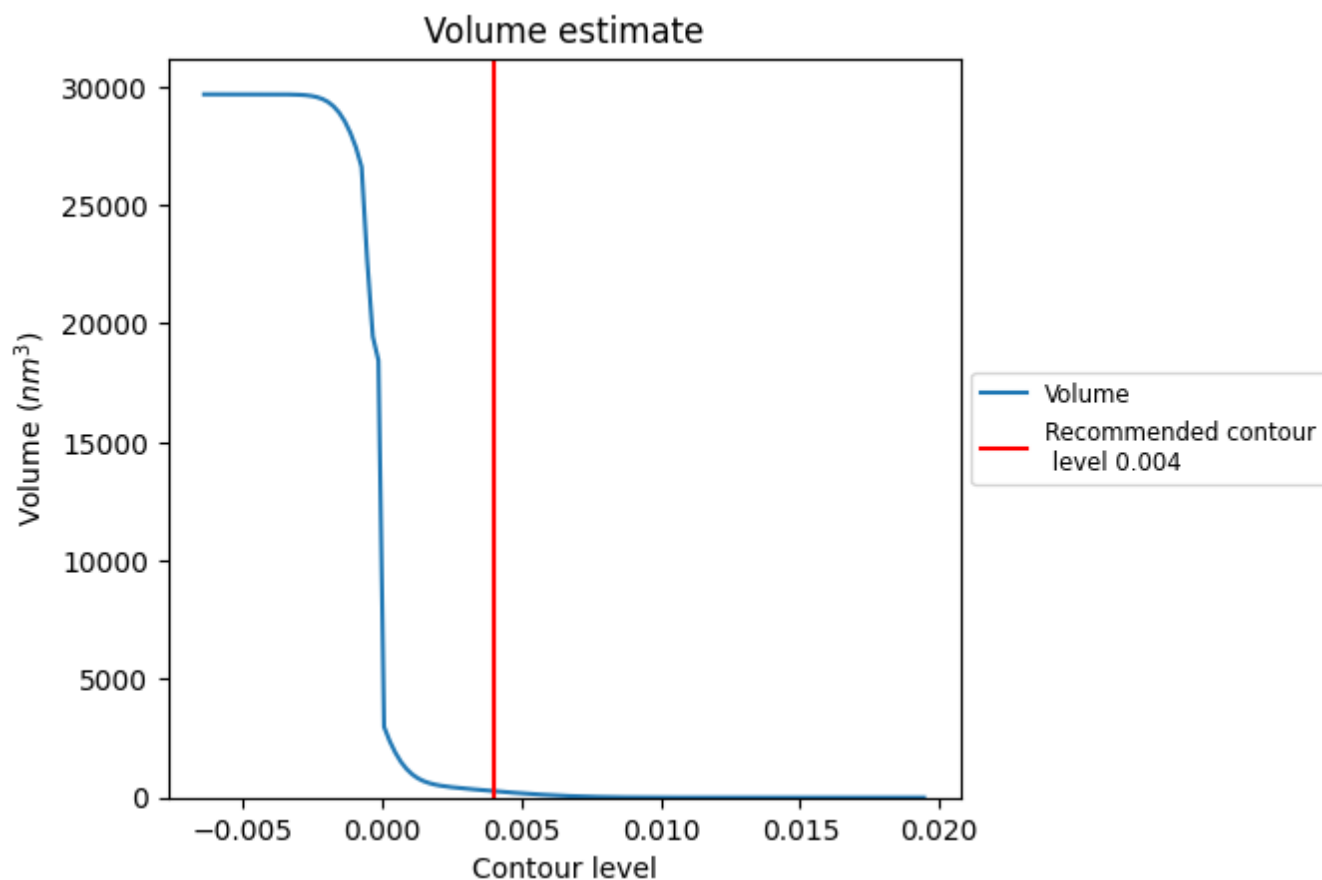
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

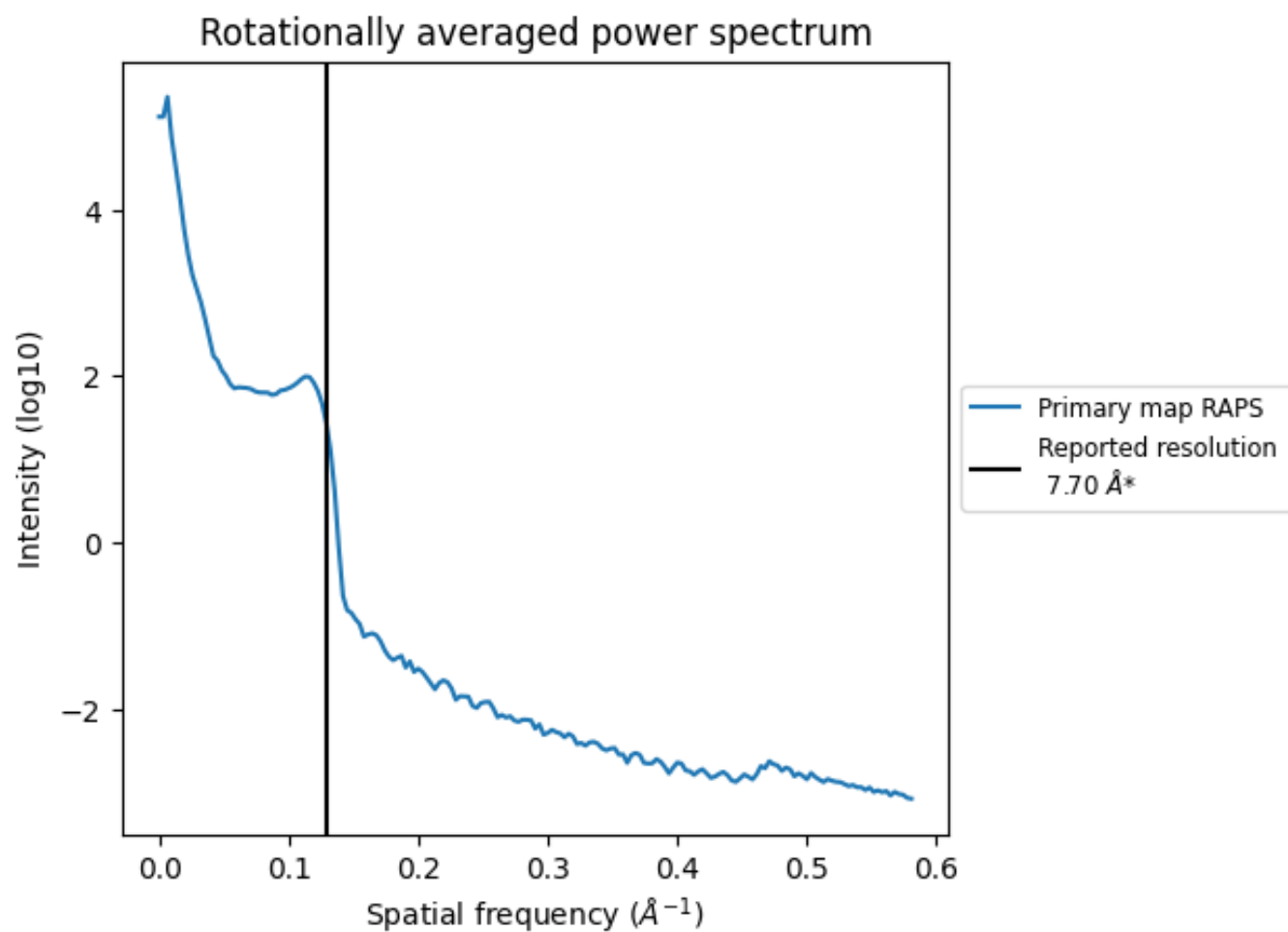
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm³; this corresponds to an approximate mass of 247 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.130 Å⁻¹

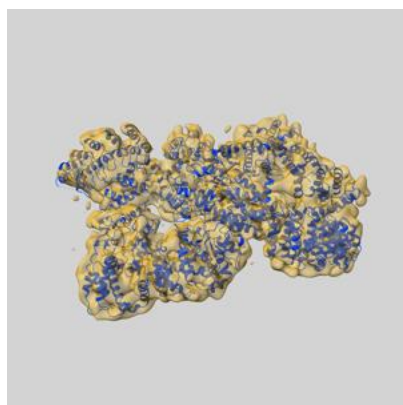
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

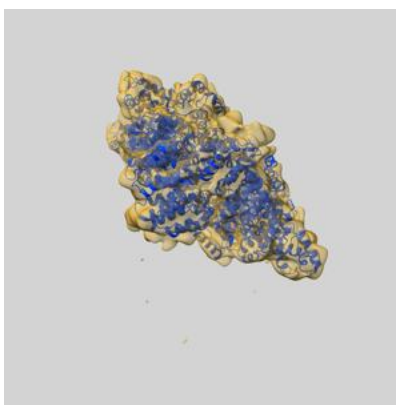
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8683 and PDB model 5VHR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

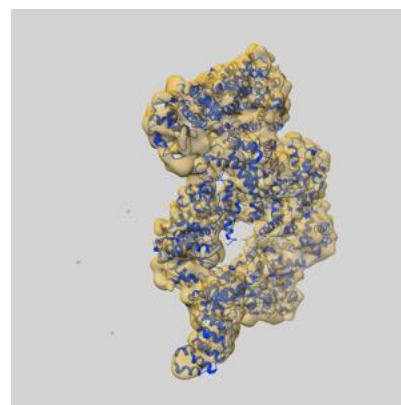
9.1 Map-model overlay [i](#)



X



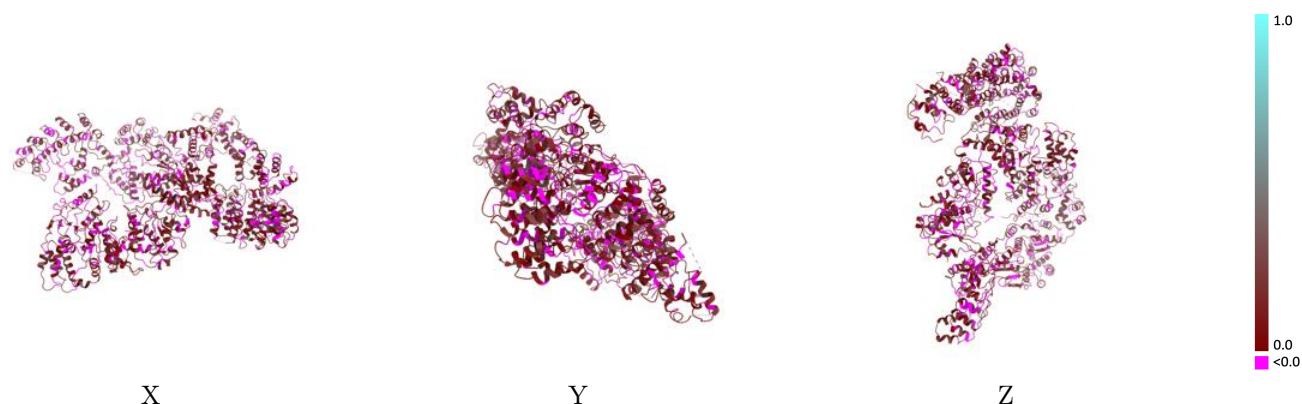
Y



Z

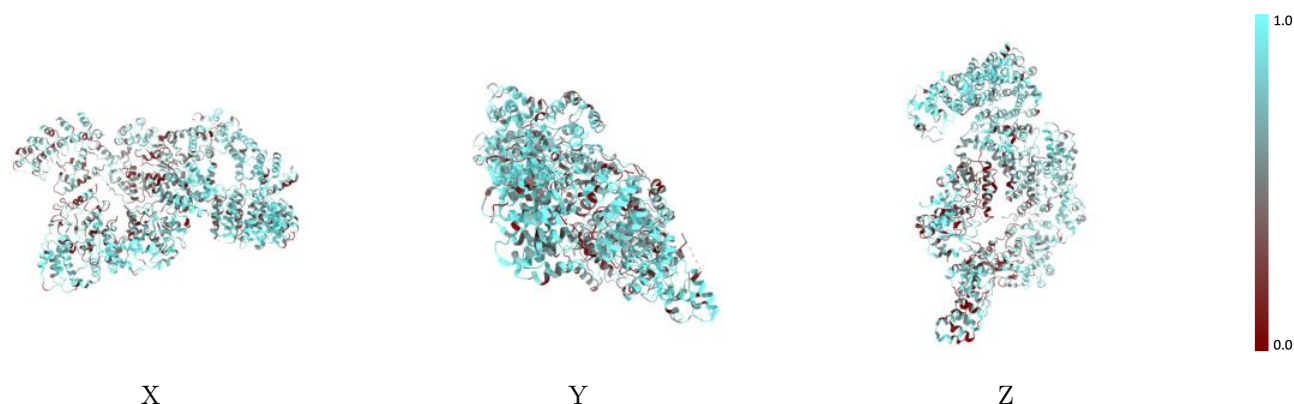
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



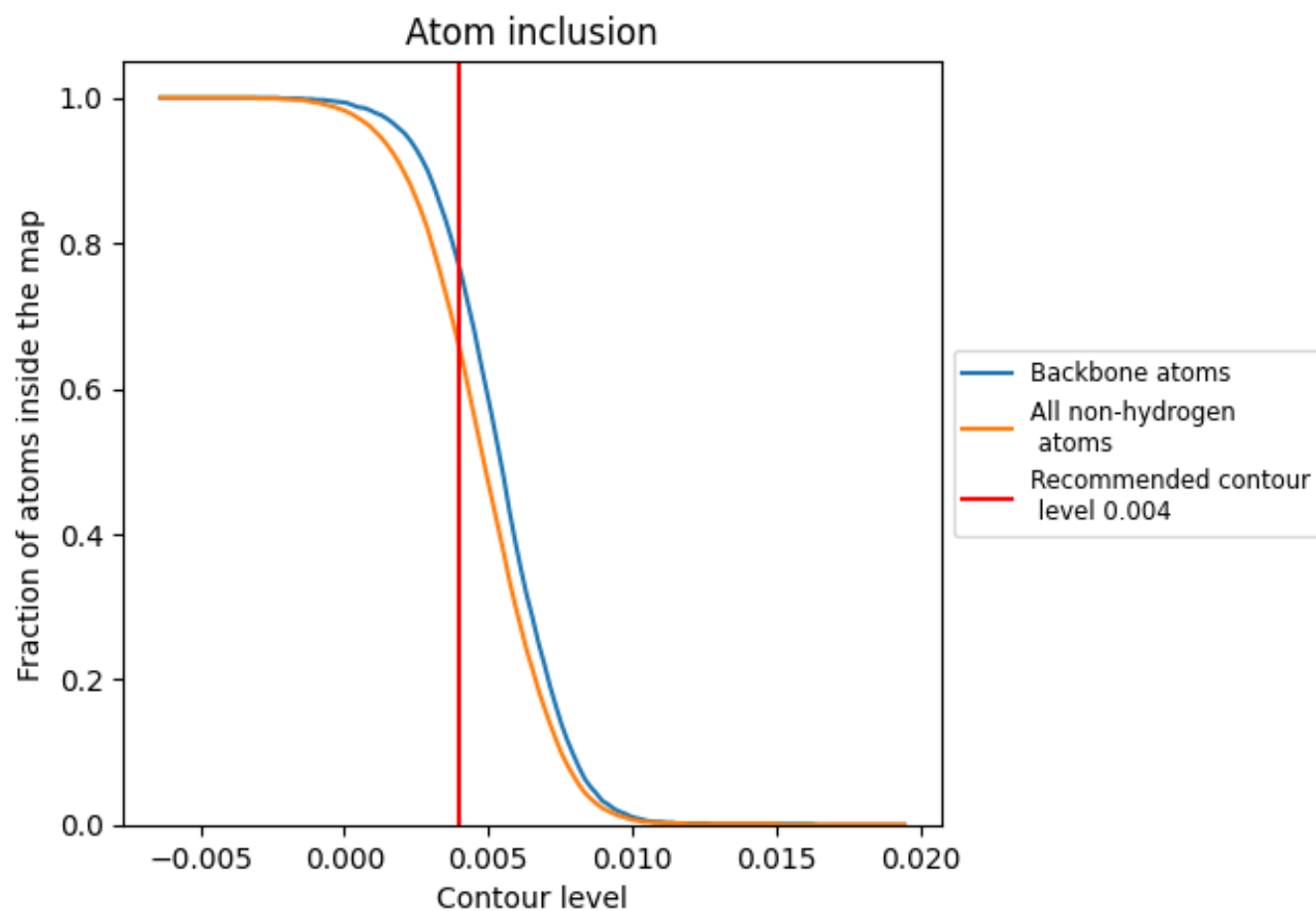
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6550	0.0920
A	0.6650	0.1040
B	0.6440	0.1070
C	0.5100	0.0870
D	0.5130	0.0600
E	0.5980	0.0770
F	0.7150	0.1010
G	0.5870	0.0860
f	0.7720	0.0990

1.0

0.0

<0.0